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SOP for Generation of Regions of Responsibility Using Dual-Energy CT

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Lawrence Livermore National Laboratory Global Security Principal Directorate **Image Database Development Project**	**Standard Operating Procedure**	
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SOP for Generation of Regions of Responsibility Using Dual-Energy CT	
Concurrence Technical Leader	Date
Approval IDD Project Principal Investigator	Date

1.0 Introduction

1.1 The purpose of this SOP is to specify the procedure used to define a Region of Responsibility (ROR) for a particular explosive material in a specified feature space scanned on a dual energy CT system.

1.2 This SOP describes the procedure used to define an ROR for at least three specimens and each has been scanned on the same dual energy CT system following the appropriate data acquisition SOP. The features of interest are μ_{high}, μ_{low}, Z_{eff}, and bulk physical density and have either been measured experimentally (in the case of bulk physical density) or extracted by the data processing method given in the appropriate analysis SOP (for μ_{high}, μ_{low} and Z_{eff}). The limits specified for the ROR are the two-sided tolerance limits for a Gaussian distribution defined such that we have 90% confidence that the feature will be inside the limits 90% of the time [Natrella, NIST Website]. To determine whether the feature distributions are Gaussian, tests such as those given in [Wikipedia Page] may be used.

2.0 References

2.1 [Natrella] M. G. Natrella, *Experimental Statistics*, National Bureau of Standards Handbook 91, 1963. Two sided tolerance limits are explained in section 2-5 and multiplicative factors K are tabulated in table A-6.

2.2 [NIST Website] http://www.itl.nist.gov/div898/handbook/prc/section2/prc263.htm

2.3 [Schneberk] D. J. Schneberk, H. E. Martz, Jr., W. D. Brown, “Home Made Explosives X-rayAttenuation: Data Analysis and Reduction of Tyndall Data: CT Systems and Pelican Case Scans,” UCRL-TR-231699, p. 11, July 2007.

2.4 [Wikipedia Page] http://en.wikipedia.org/wiki/Q%E2%80%93Q_plot

3.0 Definitions

CT	Computed Tomography. A process by which the X-ray attenuation feature of a material may be measured. This may be performed at a single energy or multiple energies.
Feature	A measurable property of a material. While this should be a property that is measurable using X-ray CT (e.g. attenuation, Z_{eff}, Ratio of μ_{low}/μ_{high}), it could also be, e.g., bulk physical density, color, or taste.
Feature Space	A potentially multi-dimensional space in which the ROR is defined. The limits of the ROR for each dimension are computed and specified independently of all other dimensions.
ID	Image Database
kV	kilovolts (thousands of volts).
LAC	Linear Attenuation Coefficient – a quantity characterizing how easily a material is penetrated by X-rays.
Material	The particular material for which the ROR is being defined.
Multiplier, K	The sample number dependent multiplier used to scale feature standard deviations to form two-sided tolerance limits
PI	Principal Investigator or responsible individual
ROR	Region of Responsibility. This defines the portion of the specified feature space in which the vendor is responsible for finding the particular explosive material.
Sample	A sample of the particular material for which the ROR is being defined.
SOP	Standard Operating Procedure.
Specimen	A prepared sample of material in a container which is able to be scanned on the CT system.
Two-Sided Tolerance Limits	Limits such that a chosen proportion P (at least) of the specimens will have the feature within the limits with a chosen confidence γ. P and γ are both set at 0.9.
Z_{eff}	Effective atomic number. This feature is related to the attenuation of the material as a function of X-ray energy.
$^{LW}Z_{eff}$	Effective atomic number. This feature is related to the attenuation of the material as a function of X-ray energy. The LW superscript indicates that the Livermore method of computing Z_{eff} is used and the lower energy data are beam hardening compensated using water.
μ	The mean value of the LAC over a volume of interest for a given X-ray source voltage, filtration and collimation.
μ_{high}	Mean high energy LAC for the specimen.
μ_{low}	Mean low energy LAC for the specimen.

4.0 Responsibilities and Authority

4.1 Roles:

4.1.1 LLNL: Honest Broker, X-ray Physics SME

4.1.2 TAFL: HME data collection synthesis lab

4.1.3 TSL: Conventional and Military data collection synthesis lab

4.1.4 TSA/OSC: End user of data collected under this program

4.1.5 EXD: Technical oversight and data collection process manager

4.2 The HME Working Group has the overall responsibility and authority for this procedure.

4.3 Original Standard Operation Procedures shall have the signature form completed prior to the effective date.

4.4 Laboratories (e.g. LLNL, TAFRL and TSL) using this SOP to generate RORs are responsible for assuring the quality of the data used and checking the results before using the resultant RORs.

5.0 Safety

6.0 Procedure

6.1 Extract and tabulate the features of interest from the specimen characterization spreadsheets. This will include the specimen name, and several of the following (depending on what data is available): μ_{high} , Z_{eff} , μ_{low} , μ_{low} / μ_{high}, density.

6.2 Compute and tabulate the number of samples, sample mean and standard deviation for each feature.

6.2.1 The number of specimens is a count of the number of data files , and is computed using the excel function count().

6.2.2 The sample mean of feature $\boldsymbol{X}$,$\bar{\boldsymbol{X}}$, is given by:

6.2.3 $\bar{X} = \frac{1}{n}(\sum_{i=1}^{n} X_i)$

6.2.4 and is computed using the excel function average( ).

6.2.5 The sample standard deviation of feature X, s, is given by

6.2.6 $\sigma = \sqrt{\frac{n\sum_{i=1}^{n} X_i^2 - (\sum_{i=1}^{n} X_i)^2}{n(n-1)}}$

6.2.7 and is computed using the excel function stdev( ).

6.3 Using the table below (excerpted from [Natrella] Table 6), look up the multiplier, K, for the two-sided tolerance limits for Gaussian distributions based on 90% confidence that 90% of the time the value will be within the tolerance limits. If the number of specimens exceeds those listed in the table, compute K using the information on the NIST Website. Record this value.

Number of Specimens	Multiplier, K, for Two-Sided 90:90 Tolerance Limits
2	15.978
3	5.847

4	4.166
5	3.494
6	3.131
7	2.902
8	2.743
9	2.626
10	2.535

6.4 Generate the two-sided tolerance limits for each feature and create a table with one row per feature showing the derived limits. This table describes the ROR.

6.4.1 The Lower Limit, X_L, is given by $X_L = \bar{X} - K\sigma$, where $\bar{X}$ is the feature mean, K is the multiplier, and σ is the feature standard deviation.

6.4.2 The Upper Limit, X_U, is given by $X_U = \bar{X} + K\sigma$, where $\bar{X}$ is the feature mean, K is the multiplier, and σ is the feature standard deviation.

6.5 Create a plot showing the limits of the ROR and the locations of the contributing data points. The X and Y axes will be determined by the features used in the study. Each specimen that was used should have a different symbol on the plot and the limits should be plotted as a box enclosing the ROR. The corners of the box should be (min limit feature 1, min limit feature 2), (max limit feature 1, min limit feature 2), (max limit feature 1, max limit feature 2), and (min limit feature 1, max limit feature 2). Two examples are given in Appendix A.

6.6 Save the resulting tables and plots and record the results. Give these to the PI.

7.0 Document Revision History

Date	Revision	Author	Responsible Manager	Comments
11/12/2013	Rev #0	Jeffrey S. Kallman	Harry E. Martz, Jr.	Converted MCT version of ROR Generation SOP to be system independent
11/25/2013	Rev # 1	Harry E. Martz, Jr.	Harry E. Martz, Jr.	Removed MCT, added PI and ID in definitions, made a few editorial comments.
12/2/2013	Rev #2	Jeffrey S. Kallman	Harry E. Martz, Jr.	Changed revision and version numbers
4/21/2014	Rev #3	Jeffrey S. Kallman	Harry E. Martz, Jr.	Incorporated roles

Appendix A: Examples

Example #1 – Generating an ROR using μ_{high} and $^{LW}Z_{eff}$

As a first example, consider generating an ROR in (μ_{high}, $^{LW}Z_{eff}$) space using three recent water specimens scanned at TAFRL.

Section 6.1: Gather the characterization spreadsheets for each of the material specimens that will be used to formulate the ROR

The specimen characterizations are stored on the DHS ID server at:

- LEDP_Active:\TP35_Industrial_CT_of_HME\Tyndall\None\Yxlon\None\130610_Water\H2O BHC\H2O BHC_analysis_INITIALS_130610\H2O BHC_characterization.xlsx
- LEDP_Active:\TP35_Industrial_CT_of_HME\Tyndall\None\Yxlon\None\130614_Water\H2O BHC\H2O BHC_analysis_INITIALS_130614\H2O BHC_characterization.xlsx
- LEDP_Active:\TP35_Industrial_CT_of_HME\Tyndall\None\Yxlon\None\130708_Water\H2O BHC\H2O BHC_analysis_INITIALS_130708\H2O BHC_characterization.xlsx

Section 6.2: Extract and tabulate the features of interest from the characterization spreadsheets. This will include the specimen name, μ_{high} , and $^{LW}Z_{eff}$.

The μ_{high} and $^{LW}Z_{eff}$ features are in cells C2 and H24 respectively in each spreadsheet. They are assembled in the following table:

Specimen	μ_{high}	$^{LW}Z_{eff}$
130610_Water	1014.016	7.555
130614_Water	1013.368	7.581
130708_Water	1012.388	7.577

Section 6.2 continued: Compute and tabulate the number of samples, sample mean and standard deviation for each feature.

These values were calculated using excel.

Water	Number of Specimens	Mean	Standard Deviation
μ_{high}	3	1013.257	0.819623
$^{LW}Z_{eff}$	3	7.571	0.014

Section 6.3: Using the table below (excerpted from [Natrella] Table 6), look up the multiplier, K, for the two-sided tolerance limits for Gaussian distributions based on 90% confidence that 90% of the time the value will be within the tolerance limits. Record this value.

Number of Specimens	Multiplier, K, for Two-Sided 90:90 Tolerance Limits
2	15.978
3	5.847

4	4.166
5	3.494
6	3.131
7	2.902
8	2.743
9	2.626
10	2.535

There are three specimens that make up the data set, so the factor K for Two-sided 90:90 tolerance limits is 5.847.

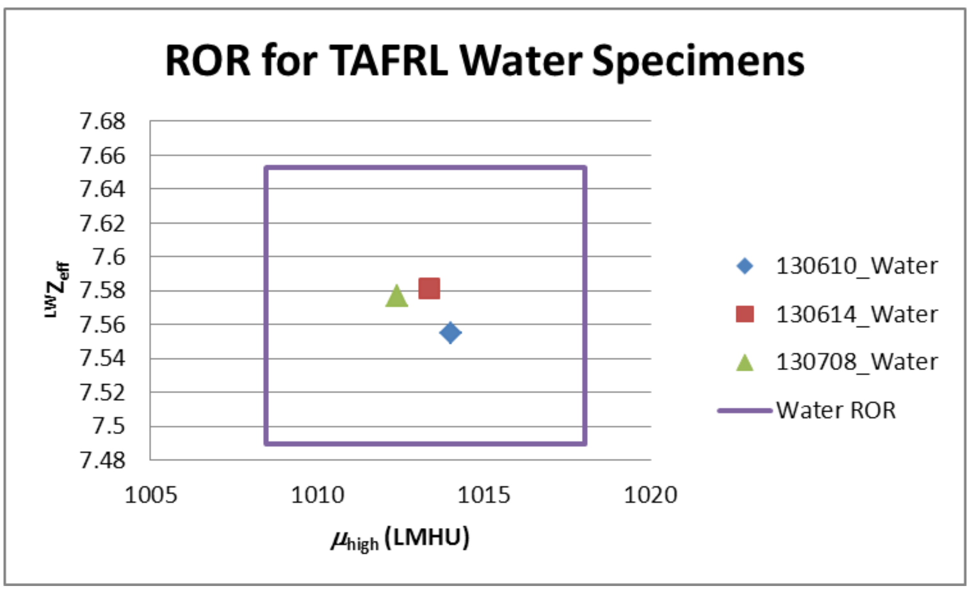
Section 6.4: Generate the two-sided tolerance limits for each feature and create a table with one row per feature showing the derived limits.

Example (μ_{high}) Lower Limit: X_L =1013.257-(5.847*0.8196)=1008.465

Example (μ_{high}) Upper Limit: X_U =1013.257+(5.847*0.8196)=1018.05

Water	Lower Limit	Upper Limit
μ_{high}	1008.05	1018.465
$^{LW}Z_{eff}$	7.489	7.653

Section 6.5: Create a plot showing the limits of the ROR and the locations of the contributing data points. The X and Y axes will be determined by the features used in the study. Each specimen that was used should have a different symbol on the plot and the limits should be plotted as a box enclosing the ROR. The corners of the box should be (min limit feature 1, min limit feature 2), (max limit feature 1, min limit feature 2), (max limit feature 1, max limit feature 2), and (min limit feature 1, max limit feature 2).



Example #2 – Generating an ROR using Density and $^{LW}Z_{eff}$

Consider generating an ROR in (density, $^{LW}Z_{eff}$) space using nine specimens of Tartaric Acid scanned at LLNL[1].

Section 6.1: Gather the characterization spreadsheets for each of the material specimens that will be used to formulate the ROR

The specimen $^{LW}Z_{eff}$ feature is stored in the characterization spreadsheets as in the first example above. In this case the density information was stored in the chemist's notes for each specimen. The specimen characterizations are stored on the DHS ID server at:

- X:\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LP02_130702\Analyses\TA_LP02_130702_H2O-BHC_analysis_IMS_130702\TA_LP02_130702_H2O-BHC_characterization.xlsx
- X:\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LP03_130703\Analyses\TA_LP03_130703_H2O-BHC_analysis_IMS_130703\TA_LP03_130703_H2O-BHC_characterization.xlsx
- X:\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LP04_130708\Analyses\TA_LP04_130708_H2O-BHC_analysis_IMS_130710\ TA_LP04_130708_H2O-BHC_characterization.xlsx
- X:\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LT02_130722\Analyses\TA_LT02_130722_H2O-BHC_analysis_IMS_130722\TA_LT02_130722_H2O-BHC_characterization.xlsx
- X:\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LT03_130723\Analyses\TA_LT03_130723_H2O-BHC_analysis_IMS_130723\TA_LT03_130723_H2O-BHC_characterization.xlsx
- X:\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LT04_130724\Analyses\TA_LT04_130724_H2O-BHC_analysis_IMS_130724\TA_LT04_130724_H2O-BHC_characterization.xlsx
- X:\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LH02_130814\Analyses\TA_LH02_130814_H2O-BHC_analysis_IMS_130814\TA_LH02_130814_H2O-BHC_characterization.xlsx
- X:\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LH03_130815\Analyses\TA_LH03_130815_H2O-BHC_analysis_IMS_130815\TA_LH03_130815_H2O-BHC_characterization.xlsx
- X:\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LH04_130822\Analyses\TA_LH04_130822_H2O-BHC_analysis_IMS_130822\TA_LH04_130822_H2O-BHC_characterization.xlsx

[1] Note that the assumption of Gaussian distribution of the features is incorrect in this situation as there are three specific packing techniques used in obtaining these data. Nevertheless, the same procedure is used. A consequence of using the same procedure is that the ROR may be wider than necessary in the non-Gaussian feature direction. Alternatively, an ROR could be generated for each packing technique and the union of the RORs could be used as the final ROR. As there would be a reduced number of samples for each packing condition, the multiplier will be larger, and the union of RORs may end up larger than the ROR generated by using the specimens together.

Section 6.2: Extract and tabulate the features of interest from the characterization spreadsheets. This will include the specimen name and $^{LW}Z_{eff}$.

The density feature is found on the second to the last line of the Acquisition Notes.txt file and the $^{LW}Z_{eff}$ feature is found in cell H24 of the characterization spreadsheet:

Specimen	Density	$^{LW}Z_{eff}$
TA_LP02_130702	0.781	7.368
TA_LP03_130703	0.770	7.363
TA_LP04_130708	0.770	7.372
TA_LT02_130722	0.889	7.373
TA_LT03_130723	0.874	7.344
TA_LT04_130724	0.888	7.374
TA_LH02_130814	0.932	7.359
TA_LH03_130815	0.945	7.404
TA_LH04_130822	0.968	7.422

Section 6.2 continued: Compute and tabulate the number of samples, sample mean and standard deviation for each feature.

These values were calculated using excel.

Tartaric Acid	Number of Specimens	Mean	Standard Deviation
Density	9	0.868556	0.077198
$^{LW}Z_{eff}$	9	7.375444	0.023644

Section 6.3: Using the table below (excerpted from [Natrella] Table 6), look up the multiplier, K, for the two-sided tolerance limits for Gaussian distributions based on 90% confidence that 90% of the time the value will be within the tolerance limits. Record this value.

Number of Specimens	Multiplier, K, for Two-Sided 90:90 Tolerance Limits
2	15.978
3	5.847
4	4.166
5	3.494
6	3.131
7	2.902
8	2.743
9	2.626
10	2.535

There are nine specimens that make up the data set, so the factor K is 2.626.

Section 6.4: Generate the two-sided tolerance limits for each feature and create a table with one row per feature showing the derived limits.

Example (Density) Lower Limit: X_L =0.868556-(2.626*0.077198)=0.6665834
Example (Density) Upper Limit: X_U =0.868556+(2.626*0.077198)=1.071277

Tartaric Acid	Lower Limit	Upper Limit
Density	0.6665834	1.071277
$^{LW}Z_{eff}$	7.313356	7.437533

Section 6.5: Create a plot showing the limits of the ROR and the locations of the contributing data points. The X and Y axes will be determined by the features used in the study. Each specimen that was used should have a different symbol on the plot and the limits should be plotted as a box enclosing the ROR. The corners of the box should be (min limit feature 1, min limit feature 2), (max limit feature 1, min limit feature 2), (max limit feature 1, max limit feature 2), and (min limit feature 1, max limit feature 2).